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An iterative method for the approximation of fibers in slow-fast systems

K. Uldall Kristiansen, M. Brøns and J. Starke

Abstract

In this paper we extend a method for iteratively improving slow manifolds so that it also can be used to approximate the fiber directions. In its original form the method was previously used successfully by the first author and C. Wulff to obtain slow manifolds, including normally elliptic ones in Hamiltonian systems, with exponentially small error-field in analytic systems. The extended method is applied to general finite dimensional real analytic systems where we obtain exponential estimates of the tangent spaces to the fibers. The method is easily implemented numerically, which we demonstrate on the Michaelis-Menten-Henri model. Finally, we extend the method further so that it also approximates the curvature of the fibers.

1 Introduction

Singularly perturbed systems involving different scales in time and/or space arise in a wide variety of scientific problems. Important examples include: meteorology and short-term weather forecasting [17, 18, 28], molecular physics and the Born-Oppenheimer approximation [21], chemical enzyme kinetics and the Michaelis-Menten mechanism [22], predator-prey and reaction-diffusion models [23], the evolution and stability of the solar system [15, 16] and the modeling of tethered satellites [29, 30]. These systems can also be “artificially constructed” by a partial scaling of variables near a bifurcation [26]. The main advantage of identifying slow and fast variables is dimension reduction by which all the fast variables are “slaved” to the slow ones through the *slow manifold*. Dimension reduction is one of the main aims and tools for a dynamicist and the elimination of fast variables is very useful in for example numerical computations. In fact, since fast variables require more computational effort and evaluations, this reduction often bridges the gap between tractable and intractable computations. An example of this is the long time (*Gyears*) integration of the solar system, see [15, 16]. See also [2] for a numerical treatment of slow-fast systems.

Slow-fast systems and singular perturbation theory. We consider slow-fast systems of the form

$$\begin{aligned}\partial_t x &= \epsilon X(x, y), \\ \partial_t y &= Y(x, y),\end{aligned}\tag{1.1}$$

with a small parameter ϵ . The vector-fields X and Y will in general also depend upon ϵ , but we shall throughout suppress this dependency. In fact, one of the advantages of the method we use is that it does not require any smoothness of X and Y as a function of ϵ . We assume that $\partial_y Y$ is invertible on the set $\{Y(x, y) = 0\}$ for $\epsilon = 0$. This is precisely the meaning of y being fast. Here ∂_z is used to denote the partial derivatives $\frac{\partial}{\partial z}$, and we will continue to use this symbol regardless of what object is being differentiated. By the implicit function theorem the set $\{Y(x, y) = 0\}$ can therefore locally be represented as a graph $M_0 = \{y = \eta_0(x)\}$, and we introduce $(x, y) = (x_0, y_0 + \eta_0(x_0))$ to transform these equations into

$$\begin{aligned}\partial_t x_0 &= \epsilon X_0(x_0, y_0), \\ \partial_t y_0 &= Y_0(x_0, y_0) = \rho_0(x_0) + A_0(x_0)y_0 + R_0(x_0, y_0),\end{aligned}\tag{1.2}$$

with

$$\rho_0 = -\epsilon \partial_x \eta X(x_0, \eta_0), \quad A_0 = \partial_y Y(x_0, \eta_0) - \epsilon \partial_x \eta \partial_y X(x_0, \eta_0),$$

$R_0(x, y_0) = \mathcal{O}(y_0^2)$ and $X_0(x_0, y_0) = X(x_0, \eta_0 + y_0)$. The manifold M_0 is not invariant since $Y_0|_{y_0=0} = \rho_0$, but it is close to being invariant as $\rho_0 = \mathcal{O}(\epsilon)$ is small.

In slow-fast systems one often connects (1.2) with the system

$$\begin{aligned}\partial_\tau x_0 &= X_0(x_0, y_0), \\ \epsilon \partial_\tau y_0 &= \rho_0(x_0) + A_0(x_0)y_0 + R_0(x_0, y_0),\end{aligned}\tag{1.3}$$

related to (1.2) by the scaling of time $\tau = \epsilon t$. If we formally set $\epsilon = 0$ in (1.2) and (1.3), then two limit systems are obtained. In (1.3), the formal limit is singular leading to the algebraic equation: $A_0(x_0)y_0 + R_0(x_0, y_0) = 0$. Note that A_0 and R_0 are here evaluated at $\epsilon = 0$. Due to the singular nature of this limit the theory is also referred to as singular perturbation theory. The set of points $M_0 = \{y_0 = 0\}$ satisfying these equations is called a *slow manifold* in the sense of MacKay [20], Definition 1, (or a critical manifold [11]) and the corresponding system: $\partial_\tau x_0 = X_0(x_0, 0)$ is called *the slow subsystem*.¹ On the other hand, in (1.2), the formal limit leads to *the fast sub-*, or *frozen*, system: $\partial_t y_0 = A_0(x_0)y_0 + R_0(x_0, y_0)$ with x_0 now considered as a parameter. In this system, M_0 is a set of equilibria and the linearization $\partial_\tau \delta y_0 = A_0(x_0)\delta y_0$ about these determine the classification of the slow manifold. In particular, if $y_0 = 0$ is an elliptic or hyperbolic equilibrium, then the slow manifold M_0 is said to be normally elliptic respectively hyperbolic at the point $(x_0, 0)$. If M_0 is normally elliptic and the vector-field is real-analytic then there exists an almost invariant slow manifold M_ϵ nearby. By “almost” it is understood that the error field, that is the normal component of the vector field restricted to the slow manifold, is of order $\mathcal{O}(e^{-C/\epsilon})$, $C > 0$. If the slow-fast system is Hamiltonian then M_ϵ can be made symplectic on which a (formally) reduced Hamiltonian system can be defined. These are basically the main results of [31]. These results are obtained using *the method of straightening out* which we now explain.

The SO method. We now describe the method of straightening out as it is presented by MacKay in [20]. We will henceforth abbreviate this method by SO. It is this method which we in this manuscript seek to extend. The method is iterative, considering normal forms of the form (1.2) at each step of the iteration. To complete the first step of the iteration, consider the equation $Y_0 = 0$, with Y_0 as in (1.2). This gives, by applying the implicit function theorem, a solution $y_0 = \eta_1(x_0)$ close to

$$\eta_1 \approx -A_0^{-1} \rho_0, \quad (1.4)$$

since $R_0 = \mathcal{O}(y_0^2)$. The graph $M_1 = \{y_0 = \eta_1(x_0)\}$ will be an improved slow manifold. To show that this is indeed an improved slow manifold, one *straightens out* the new slow manifold by introducing y_1 through $y_0 = y_1 + \eta_1$. Then the equations become

$$\partial_t x_0 = \epsilon X_1(x_0, y_1), \quad \partial_t y_1 = Y_1(x_0, y_1) = \rho_1(x_0) + A_1(x_0)y_1 + R_1(x_0, y_1),$$

with

$$\rho_1 = -\epsilon \partial_x \eta_1 X_0(x_0, \eta_1), \quad (1.5)$$

and so formally $\rho_1 = \mathcal{O}(\epsilon^2)$, since $\eta_1 = \mathcal{O}(\epsilon)$ (1.4), which is the measure of the error-field, an improvement from $\mathcal{O}(\epsilon)$ to $\mathcal{O}(\epsilon^2)$. Here $Y_1 = -\epsilon \partial_x \eta_0 X_0(x_0, y_1 + \eta_1) + Y_0(x_0, y_1 + \eta_1)$ and $X_1 = X_0(x_0, y_1 + \eta_1)$. We use $\partial_x \eta$ rather than $\partial_{x_0} \eta$ to avoid clutter. Continuing in this way, at each step solving $Y_i(x_0, y_i) = 0$ for $y_i = \eta_{i+1}(x_0)$ and then setting $y_i = y_{i+1} + \eta_{i+1}(x_0)$, we obtain an improved error at the end of each step which is a $\mathcal{O}(\epsilon)$ -multiple of the previous error leading to formal $\mathcal{O}(\epsilon^n)$ -estimates. The method, though viewed slightly differently, is actually identical to the method suggested by Fraser and Roussel [6, 27]. In [12] this method

¹Often slow manifolds are also required to be invariant, but this is too strong a requirement in the normally elliptic setting. This is the motivation for MacKay’s definition.

is also referred to as the iterative method of Fraser and Roussel. This can be realized by introducing the partial sum $\eta^n = \sum_{i=1}^n \eta_i$ and expanding $Y_{n-1}(x_0, \eta_n(x_0))$ as

$$\begin{aligned} Y_{n-1}(x_0, \eta_n(x_0)) &= -\epsilon \partial_x \eta_{n-1} X_{n-2}(x_0, \eta_{n-1} + \eta_n) + Y_{n-2}(x_0, \eta_{n-1} + \eta_n) \\ &= -\epsilon \partial_x \eta_{n-1} X_{n-3}(x_0, \eta_{n-2} + \eta_{n-1} + \eta_n) - \epsilon \partial_x \eta_{n-2} X_{n-3}(x_0, \eta_{n-2} + \eta_{n-1} + \eta_n) \\ &\quad + Y_{n-3}(x_0, \eta_{n-2} + \eta_{n-1} + \eta_n) = \cdots \\ &= -\epsilon \partial_x \eta^{n-1} X_0(x_0, \eta^n) + Y_0(x_0, \eta^n). \end{aligned}$$

The equation:

$$-\epsilon \partial_x \eta^{n-1} X_0(x_0, \eta^n) + Y_0(x_0, \eta^n) = 0, \quad (1.6)$$

defines the n th step of Fraser and Roussel's iterative method in which one solves for an improved slow manifold η^n , see [6, 27] and [12] where an asymptotic analysis of the method is given. The reference [12] does, however, not obtain exponential estimates. When the method is viewed within MacKay's setting we can also realize that we can in fact allow A_0 to be an unbounded operator: It is only necessary to assume that $A_0(x)^{-1}$ is bounded, making the approach potentially useful for partial differential equations. Note that ρ_1 actually vanishes at a true equilibrium where $X_0(x_0, \eta_0) = 0$, and the improved slow manifold $M_1 = \{y_1 = 0\}$ therefore includes all equilibria near M_0 . This property is preserved when using the method iteratively.

For Neishtadt's Hamiltonian example

$$H = \frac{1}{2}x^2 + \frac{1}{2}y^2 + v + \epsilon y f(u),$$

with $f(u) = \sum_{n=1}^{\infty} e^{-n} \sin(nu)$ and symplectic form $\omega = dx \wedge dy + \epsilon^{-1} du \wedge dv$, one can by introducing $\zeta = x + iy$ construct the optimal slow manifold and show that it cannot be improved beyond an exponential estimate. See [8]. The almost invariance is therefore the best one can aim for in a general setting for normally elliptic slow manifolds. Normally hyperbolic slow manifolds, on the other hand, persist. Nevertheless, it is not in general possible to show convergence of the iteration. This is due to the fact that the persistent manifolds, as with center manifolds, are not in general analytic [1].

Normally hyperbolic slow manifolds and their fibers. When M_0 is normally hyperbolic then Fenichel's theory [4, 5] applies and there exists a perturbed, invariant slow manifold M_ϵ for $\epsilon \neq 0$ nearby. Moreover, the stable and unstable manifolds persist. To explain the latter, consider at $\epsilon = 0$ the fast fiber $F_0^{z_0} = \{(x_0, y_0) \mid \|y_0\| \leq \Delta\}$ based at the point $z_0 = (x_0, 0)$. If the real parts of the eigenvalues of A are all negative, then M_0 for $\epsilon = 0$ is asymptotically stable and all solutions on $F_0^{z_0}$ contract exponentially toward the base point z_0 provided Δ is sufficiently small. By Fenichel's theory the fast fibers $F_0^{z_0}$ perturb to $F_\epsilon^{z_0}$ forming an invariant family $F_\epsilon = \cup_{z_0 \in M_\epsilon} F_\epsilon^{z_0}$ along which solutions contract to M_ϵ . The invariance of this family is understood in the following sense

$$\Phi_0^t(F_\epsilon^{z_0}) \subset F_\epsilon^{\Phi_0^t(z_0)},$$

where Φ_0^t is the time- t flow map of (1.2). The motion of any point on $F_\epsilon^{z_0}$ therefore decomposes into a fast contracting component and a slow component governed by the motion of the base

point $z_b = \pi_f z$ of the fiber. In the physics literature a fiber is also sometimes called an isochron [3].

The fiber projection π_f is smooth, and so locally there exists a transformation $(u, v) \mapsto (x_0, y_0)$, which is $\mathcal{O}(\epsilon)$ close to the identity, mapping (1.2) into the Fenichel normal form [11]:

$$\partial_t u = \epsilon U(u), \quad \partial_t v = V(u, v)v.$$

These are the ideal coordinates for the description of the system near the slow manifold, in particular useful when solving the problem numerically; the slow manifold coincides with the zero level set $\{v = 0\}$ and the fibers of the form $F_\epsilon^{(u_*, 0)}$ have been straightened out to $\{(u, v) | u = u_*, \|v\| \leq \Delta\}$. We will approach this ideal by first constructing a transformation $(x, y) \mapsto (x_0, y_0)$ so that the x -equation, up to exponentially small error terms, becomes independent of y to linear order:

$$\begin{aligned} \partial_t x &= \epsilon(\Lambda(x) + \mathcal{O}(y^2)) + \mathcal{O}(e^{-c/\epsilon}), \\ \partial_t y &= A(x)y + \mathcal{O}(y^2) + \mathcal{O}(e^{-c/\epsilon}). \end{aligned}$$

Then the tangent space to the fibers at $(x_*, 0)$ will *almost* coincide with $\{(x, y) | x = x_*\}$. Later we will also seek to remove the terms that are quadratic in y . Similar ideas have been developed in [3, 25] for center manifolds near non-hyperbolic equilibria.

When M is of saddle type, with a stable manifold $W^s(M)$ of dimension n_f^s and an unstable manifold $W^u(M)$ of dimension n_f^u ($n_f = n_f^s + n_f^u$), then Fenichel's normal form takes a slightly different form: There exists a transformation $(u, v, w) \mapsto (x_0, y_0)$, with $\dim\{v\} = n_f^s$ and $\dim\{w\} = n_f^u$, which is $\mathcal{O}(\epsilon)$ close to the identity, mapping (1.2) into

$$\begin{aligned} \partial_t u &= \epsilon(U_0(u) + U_1(u, v, w)vw), \\ \partial_t v &= V(u, v, w)v, \\ \partial_t w &= W(u, v, w)w. \end{aligned} \tag{1.7}$$

Here $U_1(u, v, w) : \{v\} \times \{w\} \rightarrow \mathbb{R}^{n_s}$ is a bilinear function of v and w . The slow manifold is then given by $\{v = 0, w = 0\}$ with stable manifold $\{w = 0\}$ and unstable manifold $\{v = 0\}$. The transformation may only exist in a small neighborhood of the slow manifold so in general we need $\|v\| \leq \Delta_v$ and $\|w\| \leq \Delta_w$.

Reduction methods. There are several alternatives to the method of straightening out for approximating slow manifolds. We name a few others: The intrinsic low-dimensional manifold (ILDm) method of Maas and Pope [19], the zero-velocity principle (ZVP) [7, 32], and the computational singular perturbation (CSP) method initially due to Lam and Goussis [13, 14], but later extended by Zagaris and co-workers [33]. The ILDM method is based on the Jacobian of the vector-field and partitions this at each point into a fast and a slow component based on spectral gaps of the Jacobian. The ILDM approximation to the slow manifold is then defined as the locus of points where the vector-field lies entirely in the slow subspace. In general, this only gives an approximation that agrees up to $\mathcal{O}(\epsilon)$ [12]. Nevertheless, the method is still quite powerful as it can be used in systems where a small parameter may not be directly available. In the ZVP method an $\mathcal{O}(\epsilon^n)$ -approximation to the slow manifold is obtained as the locus of points where the $(n + 1)$ th time derivative of the fast variable vanishes. This method has been used in an equation-free setting in [7].

A distinctive contribution of the CSP method is that it also approximates the fibers in the sense that it provides a set of basis vectors spanning the tangent spaces of the fibers at the slow manifolds up to $\mathcal{O}(\epsilon^n)$. We will in this paper show that it is also possible to approximate these tangent spaces by adding an extra step to the method of straightening out. The transformations we use have direct interpretations, and the method can be formulated in a way that is similar to how Fraser and Roussel presented the method of straightening out, only involving evaluations of the initial vector-field and its Jacobian matrix. Finally, the method can be further extended so that it also approximates the curvature of the fibers. In principle higher order effects can also be accounted for, but this introduces a certain degree of complexity. In this paper we will therefore focus most of our effort on demonstrating the first part of the method which seeks to estimate the tangent spaces of the slow manifold. Once this approach has been established and demonstrated on the Michaelis-Menten-Henri model, we will consider removing the part of the slow vector-field which is quadratic in the fast variable, hence approximating the curvature of the fibers. One of the reasons for choosing the Michaelis-Menten-Henri model as our example is that all the calculations can be done explicitly. But moreover, it also allows for comparison with the results in [33] from the application of the CSP method.

The SOF method. In this section we shortly describe our method for approximating the tangent spaces of the fibers. We will refer to this method as the *SOF method* - the extra F has been added to SO to indicate that the approximation of the fiber directions is build in as an extension of the original SO method. The method is based on normal form computations, see e.g. [9] section 3.3. We start from the real analytic slow-fast system:

$$\begin{aligned}\partial_t x_0 &= \epsilon X(x_0, y) = \epsilon(\Lambda(x_0) + \mu_0(x_0)y + T(x_0, y)), \\ \partial_t y &= Y(x_0, y) = \rho(x_0) + A(x_0)y + R(x_0, y),\end{aligned}$$

with ρ describing the error-field on $\{y = 0\}$ and $R, T = \mathcal{O}(y^2)$. We assume that there are n_s slow variables $x \in \mathbb{R}^{n_s}$ and n_f fast variables $y \in \mathbb{R}^{n_f}$. Following the $\mathcal{O}(\epsilon^{-1})$ applications of the SO method we can take $\rho = \mathcal{O}(e^{-c/\epsilon})$ [31], and for the purpose of obtaining exponential estimates we can therefore ignore this term completely. The aim is to introduce a succession of transformations of the form $x_i = x_{i+1} + \epsilon\phi_i(x_{i+1})y$ formally pushing the term in $\epsilon^{-1}\partial_t x_{i+1}$ which is linear in y to consecutive higher order in ϵ . Let us consider the first step, introducing $x_0 = x_1 + \epsilon\phi_0(x_1)y$ so that

$$\begin{aligned}\partial_t x_1 &= J^{-1}(\epsilon\Lambda(x_0) + \epsilon\{\epsilon\partial_x\Lambda\phi_0 + \mu_0 - \phi_0A\}y + \epsilon\mathcal{O}(y^2)) \\ &= \epsilon(\Lambda + \{\epsilon\partial_x\Lambda\phi_0 + \mu_0 - \phi_0A\}y - \epsilon\partial_x\phi_0\Lambda y + \mathcal{O}(y^2))\end{aligned}\tag{1.8}$$

where $J = I_s + \epsilon\partial_x\phi_0y$, $I_s = \text{identity} \in \mathbb{R}^{n_s \times n_s}$, is the Jacobian of the transformation $x_1 \mapsto x_0$, and where we have used the identity

$$J^{-1} = I_s - \epsilon\partial_x\phi_0y + J^{-1}(\epsilon\partial_x\phi_0y)^2.$$

The term in (1.8) which is linear in y is due to two contributions. The first one is due to the expansion of $X(x_0, y) - \phi Y(x_0, y)$ in y , the curly bracket in (1.8), while the second one:

$$\mu_1 = -\epsilon\partial_x\phi_0\Lambda,\tag{1.9}$$

comes from the inverse of the Jacobian. Here $\partial_x \phi_0 \Lambda$ is understood column-wise:

$$\partial_x \phi_0 \Lambda = (\partial_x(\phi)^1 \Lambda \cdots \partial_x(\phi)^{n_f} \Lambda),$$

$(\phi)^i = (\phi)^i(x_0) \in \mathbb{R}^{n_s}$ being the i th column of $\phi = \phi(x_0) \in \mathbb{R}^{n_s \times n_f}$. We let ϕ_0 be the solution to the linear equation obtained by setting the first contribution, the curly bracket in (1.8), to zero:

$$\epsilon \partial_x \Lambda \phi_0 + \mu_0 - \phi_0 A = 0.$$

This equation has a solution ϕ_0 close to $\mu_0 A^{-1}$, and the new error term μ_1 (1.9), which by construction is the only remaining term in $\epsilon^{-1} \partial_t x_1$ linear in y , is therefore formally smaller than the old error μ_0 . There is an improvement from $\mathcal{O}(1)$ to $\mathcal{O}(\epsilon)$. Note also that

$$\Lambda_1 = \Lambda, \quad A_1 = A.$$

We will use these types of transformations successively in the proof, pushing the error term to higher order in ϵ . One of the main results of the paper is that eventually the error is exponentially small: $\mu = \mathcal{O}(e^{-c/\epsilon})$.

We present the first result formally in Theorem 2.1 which we prove in section 3. In section 4 we demonstrate how the method can be used computationally on the Michaelis-Menten-Henri model. In section 5 we present a result, Theorem 5.1, on approximation of the curvature of the fibers. Theorem 5.1 excludes normally elliptic slow manifolds and neutral saddle-type slow manifolds where both λ and $-\lambda$, $\text{Re } \lambda \neq 0$, are eigenvalues of A . This requirement appears in the construction of the appropriate transformations, where we encounter linear matrix equations of the form:

$$A^T \psi^i + \psi^i A = Q^i,$$

for the unknown matrices ψ^i . Solutions of this linear problem exist and are unique if and only if $\sigma(A) \cap \sigma(-A) = \emptyset$, see [10], Theorem 4.4.6. Here $\sigma(A)$ denotes the spectrum of the matrix A . The case where both λ and $-\lambda$, $\text{Re } \lambda \neq 0$, are eigenvalues of the A leads to small divisors, as in the problem of analytic linearization [9], and it will be considered separately in section 6.

As opposed to [31] the applications we have in mind are primarily for normally hyperbolic slow manifolds, where the fibers provide the directions of the stable and unstable manifolds along which the solutions relax to respectively escape the slow manifold. However, our results in Theorem 2.1 still hold true for the normally elliptic case by providing coordinates in which the slow dynamics become *almost* independent of the fast variables to linear order. The improved slow manifold includes all nearby equilibria and, what is also new, the Jacobian of the vector-field at an equilibrium takes a very suitable form with the linearized slow dynamics being exactly independent of the fast variables.

Notation and preliminaries. Let $(\mathcal{X}, \|\cdot\|_{\mathcal{X}})$ and $(\mathcal{Y}, \|\cdot\|_{\mathcal{Y}})$ be real Banach spaces, and $\mathcal{X}_{\mathbb{C}} = \mathcal{X} \oplus i\mathcal{X}$ respectively $\mathcal{Y}_{\mathbb{C}} = \mathcal{Y} \oplus i\mathcal{Y}$ their complexifications with norms $\|x_1 + ix_2\|_{\mathcal{X}_{\mathbb{C}}} = \|x_1\|_{\mathcal{X}} + \|x_2\|_{\mathcal{X}}$ and $\|y_1 + iy_2\|_{\mathcal{Y}_{\mathbb{C}}} = \|y_1\|_{\mathcal{Y}} + \|y_2\|_{\mathcal{Y}}$. Here we are primarily thinking of $\mathcal{X} = \mathbb{R}^{n_s}$ and $\mathcal{Y} = \mathbb{R}^{n_f}$, but other spaces will also be used and therefore prefer the general setting. As the proofs involve many transformations, we prefer to reserve the use of subscripts to

keep track of the steps in these coordinates changes, and will therefore use the alternative notation $(x)_i$, $1 \leq i \leq n$, for the i th component of a vector $x \in \mathbb{R}^n$.

We will from now on denote all norms, including operator norms, by $\|\cdot\|$. We hope that this will not cause unnecessary confusion. Hopefully it will be clear from the context what norm is used. Then $f : \mathcal{U}_{\mathbb{C}} \rightarrow \mathcal{Y}_{\mathbb{C}}$, with $\mathcal{U}_{\mathbb{C}}$ an open subset of $\mathcal{X}_{\mathbb{C}}$, is analytic if it is continuously differentiable. That is if there exists a continuous derivative $\partial_x f : \mathcal{U}_{\mathbb{C}} \rightarrow L(\mathcal{X}_{\mathbb{C}}, \mathcal{Y}_{\mathbb{C}})$, the Banach space of complex linear operators from $\mathcal{X}_{\mathbb{C}}$ to $\mathcal{Y}_{\mathbb{C}}$ equipped with the operator norm, satisfying the following condition

$$\|f(x+h) - f(x) - \partial_x f(x)(h)\| = \mathcal{O}(\|h\|^2).$$

By real analytic we will mean analytic and real when the arguments are real. The higher order derivatives can be defined inductively and $\partial_x^n f$ becomes a map

$$\partial_x^n f : \mathcal{U}_{\mathbb{C}} \rightarrow L^n(\mathcal{X}_{\mathbb{C}}, \mathcal{Y}_{\mathbb{C}}),$$

from $\mathcal{U}_{\mathbb{C}}$ into the Banach space $L^n(\mathcal{X}_{\mathbb{C}}, \mathcal{Y}_{\mathbb{C}})$ of all bounded, n -linear maps from $\mathcal{X}_{\mathbb{C}} \times \cdots \times \mathcal{X}_{\mathbb{C}}$ (n times) into $\mathcal{Y}_{\mathbb{C}}$. See [24] Appendix A for a reference on analytic function theory in Banach spaces.

When \mathcal{U} is an open subset of \mathcal{X} then we define $\mathcal{U} + i\chi$ to be the open complex χ -neighborhood of \mathcal{U} :

$$\mathcal{U} + i\chi = \{x \in \mathcal{X}_{\mathbb{C}} | d_{\mathcal{X}_{\mathbb{C}}}(x, \mathcal{U}) < \chi\},$$

where $d_{\mathcal{X}_{\mathbb{C}}}$ is the metric induced from the Banach norm $\|\cdot\|$.

We frequently need the following Cauchy estimate:

Lemma 1.1 [24] *Assume that $f : \mathcal{U}_{\mathbb{C}} \rightarrow \mathcal{Y}_{\mathbb{C}}$ is analytic and that f is bounded on the $\mathcal{X}_{\mathbb{C}}$ -open ball $B_{\xi}(x_0) \subset \mathcal{U}_{\mathbb{C}}$. Then*

$$\|\partial_x f(x_0)\| \leq \frac{\sup_{x \in B_{\xi}(x_0)} \|f(x)\|}{\xi}. \quad (1.10)$$

□

Remark 1.1 Consider $f : \mathcal{U} + i\chi \rightarrow \mathcal{Y}_{\mathbb{C}}$ analytic and bounded. Then we can apply this estimate to any $x_0 \in \mathcal{U} + i(\chi - \xi)$ to obtain:

$$\sup_{x_0 \in \mathcal{U} + i(\chi - \xi)} \|\partial_x f(x_0)\| \leq \frac{\sup_{x \in \mathcal{U} + i\chi} \|f(x)\|}{\xi},$$

which we will write compactly as

$$\|\partial_x f\|_{\chi - \xi} \leq \frac{\|f\|_{\chi}}{\xi}.$$

This is the form of Cauchy's estimate that we will be using. Similarly, we will by $\|\cdot\|_{\chi, \nu}$ denote the sup-norm taking over the domain $(\mathcal{U} + i\chi) \times (\mathcal{V} + i\nu)$ of (x, y) .

Note also that the norm on the left hand side of (1.10) is the operator norm on $L(\mathcal{X}_{\mathbb{C}}, \mathcal{Y}_{\mathbb{C}})$ of complex bounded linear operators, while the norm on the right hand side is the norm on $\mathcal{Y}_{\mathbb{C}}$. □

Remark 1.2 We write a m -linear form such as $\partial_x^m f(x) \in L^m(\mathcal{X}_{\mathbb{C}}, \mathcal{Y}_{\mathbb{C}})$ evaluated diagonally on $h \in \mathcal{X}$ as $\partial_x^m f(x)h^m$. With this notation Taylor's formula reads:

$$f(x+h) = f(x) + \partial_x f(x)h + \cdots + \frac{1}{(n-1)!} \partial_x^{n-1} f(x)h^{n-1} \\ + \int_0^1 \frac{(1-s)^{n-1}}{(n-1)!} \partial_x^n f(x+sh)h^n ds,$$

with the integral remainder being bounded by $\frac{\|h\|^n}{n!} \sup_{0 \leq s \leq 1} \|\partial_w^n f(w+sh)\|$. \square

2 Main result

We consider the real analytic slow-fast system (1.2) in the form

$$\begin{aligned} \partial_t x_0 &= \epsilon X_0(x_0, y_0) = \epsilon(\Lambda_0(x_0) + \mu_0(x_0)y_0 + T_0(x_0, y_0)), \\ \partial_t y_0 &= Y_0(x_0, y_0) = \rho_0(x_0) + A_0(x_0)y_0 + R_0(x_0, y_0), \end{aligned} \quad (2.1)$$

with n_s slow variables and n_f fast ones so that $x_0 \in \mathcal{U} + i\chi_0 \subset \mathcal{X}_{\mathbb{C}} = \mathbb{C}^{n_s}$ and $y_0 \in \mathcal{V} + i\nu_0 \subset \mathcal{Y}_{\mathbb{C}} = \mathbb{C}^{n_f}$. Here $\mathcal{U} \subset \mathcal{X} = \mathbb{R}^{n_s}$ and $\mathcal{V} \subset \mathcal{Y} = \mathbb{R}^{n_f}$ are real open subsets. Assume also that $\|\rho_0\|_{\chi_0} \leq \mathcal{O}(\epsilon)$.

Theorem 2.1 Fix $0 \leq \underline{\chi} < \chi_0$ and $0 \leq \underline{\nu} < \nu_0$. Then there exists an ϵ_0 so that for all $\epsilon \leq \epsilon_0$ the SOF method constructs a transformation $(x, y) \mapsto (x_0, y_0)$ which is ϵ -close to the identity from $(\mathcal{U} + i\underline{\chi}) \times (\mathcal{V} + i\underline{\nu})$ to $(\mathcal{U} + i\chi_0) \times (\mathcal{V} + i\nu_0)$ mapping (2.1) into

$$\begin{aligned} \partial_t x &= \epsilon(\Lambda(x) + \mu(x)y + Q(x)y^2 + C(x, y)) \\ \partial_t y &= \rho(x) + A(x)y + R(x, y) \end{aligned} \quad (2.2)$$

with μ and ρ vanishing at true equilibria,

$$\gamma = \|\mu\|_{\underline{\chi}}, \delta = \|\rho\|_{\underline{\chi}} \leq \mathcal{O}(e^{-c_1/\epsilon}),$$

and $T(x, y) = Q(x)y^2 + C(x, y)$, $C = \mathcal{O}(y^3)$,

$$\|\Lambda - \Lambda_0\|_{\underline{\chi}}, \|A - A_0\|_{\underline{\chi}}, \|T - T_0\|_{\underline{\chi}, \underline{\nu}}, \|R - R_0\|_{\underline{\chi}, \underline{\nu}} \leq c_2 \epsilon,$$

for some constants c_1 and c_2 . \square

We highlight that the estimates are not uniform in $\underline{\chi}$ and $\underline{\nu}$. We also have the following corollary which provides a convenient form for the transformation in Theorem 2.1:

Corollary 2.1 If the eigenvalues of A_0 all have non-zero real part, then there exists an ϵ_0 so that for all $\epsilon \leq \epsilon_0$ there exists a slow manifold M_ϵ of (1.2) and $N_\epsilon = \mathcal{O}(\epsilon^{-1}) \in \mathbb{N}$ so that M_ϵ is given as the graph

$$y_0 = \eta(x_0) + \mathcal{O}(e^{-C_1/\epsilon}),$$

with $\eta = \sum_{n=1}^{N_\epsilon} \eta_n$, where the partial sums $\eta^n \equiv \sum_{i=1}^n \eta_i$ satisfy (1.6) for $1 \leq n \leq N_\epsilon$ using the convention $\eta^0 \equiv 0$. Furthermore, the tangent space of the fibers $\mathcal{F}_\epsilon^{z_0}$ at the base point $z_0 = (x_0, \eta(x_0))$ is given as

$$T_{z_0} \mathcal{F}_\epsilon^{z_0} = \text{Rg} \left(\begin{pmatrix} \epsilon \phi(x_0) \\ I_f + \epsilon \partial_x \eta(x_0) \phi(x_0) \end{pmatrix} + \mathcal{O}(e^{-C_1/\epsilon}) \right). \quad (2.3)$$

Here $I_f = \text{identity} \in \mathbb{R}^{n_f \times n_f}$ and $\phi = \sum_{n=0}^{N_\epsilon} \phi_n$ where the partial sums $\phi^n = \sum_{i=0}^n \phi_i(x_0)$ satisfy

$$\epsilon(\partial_x X_0 + \partial_y X_0 \partial_x \eta) \phi^n - \epsilon \partial_x \phi^{n-1} X_0 + \partial_y X_0 - \phi^n (-\epsilon \partial_x \eta \partial_y X_0 + \partial_y Y_0) = 0, \quad (2.4)$$

for $0 \leq n \leq N_\epsilon$ using the convention $\phi^{-1} \equiv 0$. The functions X_0 , $\partial_x X_0$, $\partial_y X_0$ and $\partial_y Y_0$ are all evaluated at $(x_0, \eta(x_0))$,

PROOF Here Fenichel's theorem applies. The first part of the corollary then follows directly from [31]. For the second part, note that each ϕ_n solves (3.4) below. Here $\Lambda(x_0) = X_0(x_0, \eta(x_0))$ and $A(x_0) = -\epsilon \partial_x \eta \partial_y X_0(x_0, \eta) + \partial_y Y_0(x_0, \eta)$ from which (2.4) follows by summation over n . Also since the method generates a transformation of the form

$$x_0 = x + \epsilon \phi(x) y + \mathcal{O}(y^2), \quad y_0 = y + \eta(x_0).$$

we obtain a tangent vector to the curve $\theta = \theta((y)_i)$ at $(x_0, \eta(x_0))$ as

$$\theta'(0) = \begin{pmatrix} \epsilon(\phi)^i \\ e_i + \epsilon \partial_x \eta(\phi)^i \end{pmatrix}.$$

Also $(e_i)_j = \delta_{ij}$ Kronecker's delta, and $(\phi)^i = (\phi)^i(x_0) \in \mathbb{R}^{n_s}$ is the i th column of $\phi = \phi(x) \in \mathbb{R}^{n_s \times n_f}$. ■

We believe that these results, in particular in the form presented in Corollary 1, are useful in computations as the approximation of the relevant objects, the slow manifold and its tangent spaces, only require evaluations of the initial vector-field and its gradients. In particular, we believe that the approximations of the tangent spaces can be usefully applied in examples with many fast degrees of freedoms where one is faced with having to trade off accuracy with minimizing computational effort. From a given initial condition (x_0, y_0) , near the slow manifold, one can approximate the fiber projection $\pi_f : (x_0, y_0) \mapsto (x_b, \eta(x_b))$, onto the base point, by solving the equations

$$\begin{aligned} x_0 &= x_b^{\text{app}} + \epsilon \phi(x_b^{\text{app}}) y, \\ y_0 &= y + \eta(x_0), \end{aligned} \quad (2.5)$$

for y and x_b^{app} . The second equation gives $y = y_0 - \eta(x_0)$ which inserted into the first equation gives a non-linear equation for x_b^{app} . The right hand side of this equation is, however, ϵ -close to the identity. In [33] it is stated that this projection is only $\mathcal{O}(\epsilon)$, and therefore asymptotically in ϵ not better than the “naive projection” $(x_0, y + \eta(x_0)) \mapsto (x_0, \eta(x_0))$.

However, this estimate is for fixed y . We believe it is more appropriate to highlight that the error is of the form:

$$\|\pi_f(x_0, y_0) - (x_b^{\text{app}}, \eta(x_b^{\text{app}}))\| = \mathcal{O}(\epsilon y^2).$$

In particular it is exact (up to the exponentially small error terms) if the tangent space is a hyperplane (which [33] also highlights). The different projections are illustrated in Fig. 1. The linear projection accounts for the “initial slip” [3] along the slow manifold.

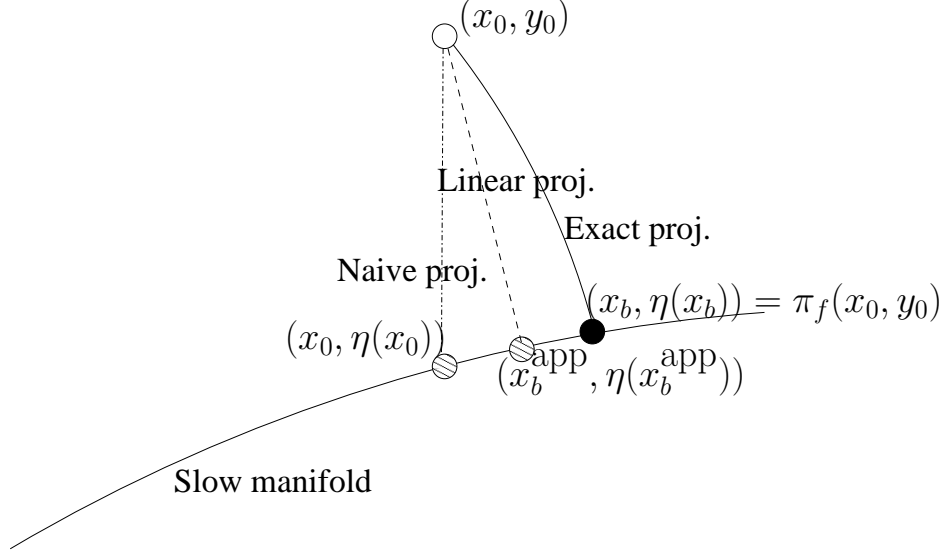


Figure 1: Illustration of the different projections: naive, linear and exact. The linear projection $(x_0, y_0) \mapsto (x_b^{\text{app}}, \eta(x_b^{\text{app}}))$ is given by the equations in (2.5).

By approximating the fiber projection we can compute approximations to the dynamics having only to propagate initial conditions on $\mathcal{O}(1)$ time scales, splitting the problem into first propagating the base point $x_b = x_b(\tau)$, $\tau = \epsilon t$, through

$$\partial_\tau x_b = X_0(x, \eta(x_b)),$$

and then follow this by propagating $y_0 = y_0(t)$ through

$$\partial_t y_0 = Y_0(x_0, y_0 + \eta(x_0)),$$

using $x_0 = x_b + \epsilon \phi(x_b)y$ and the solution $x_b = x_b(\tau)$ obtained from the first step. We aim to investigate our results within this setting in future research.

3 Proof of Theorem 2.1

We first make use of the result from [31], to transform (2.1) into

$$\begin{aligned} \partial_t x_0 &= \epsilon X(x_0, y) = \epsilon(\Lambda(x_0) + \mu_0(x_0)y + T(x_0, y)), \\ \partial_t y &= Y(x_0, y) = \rho(x_0) + A(x_0)y + R(x_0, y), \end{aligned}$$

defined on the domain $(x_0, y) \in (\mathcal{U} + i\chi) \times (\mathcal{V} + i\nu)$ with $\chi = (\underline{\chi} + \chi_0)/2$ and $\nu = \underline{\nu}$, and where $\rho = \mathcal{O}(e^{-C_1/\epsilon})$. In fact, we initially ignore this term setting $\rho \equiv 0$. Furthermore, X and Y are ϵ -close to X_0 respectively Y_0 being given by

$$\begin{aligned} X(x_0, y) &= X_0(x_0, \eta(x_0) + y), \\ Y(x_0, y) &= -\partial_x \eta X_0(x_0, \eta(x_0) + y) + Y_0(x_0, \eta(x_0) + y). \end{aligned} \quad (3.1)$$

Let K and C'_Λ be so that $\|A^{-1}\|_\chi \leq \frac{K}{2}$ and $\|\partial_x \Lambda\|_\chi \leq C'_\Lambda$.

We define the error γ_0 by

$$\gamma_0 = \|\mu_0\|_\chi,$$

and apply the transformation

$$x_0 = x_1 + \epsilon \phi_0(x_1)y,$$

where ϕ_0 solves

$$\epsilon \partial_x \Lambda \phi_0 + \mu_0 - \phi_0 A = 0. \quad (3.2)$$

Cf. (1.8) this transforms the system into

$$\begin{aligned} \partial_t x_1 &= \epsilon(\Lambda(x_1) + \mu_1 y + T_1(x_1, y)) \\ \partial_t y &= A(x_1)y + R_1(x_1, y), \end{aligned}$$

with

$$\mu_1 = -\epsilon \partial_x \phi_0 \Lambda.$$

Remark 3.1 The modified function μ_1 vanishes at an actual equilibrium where $\Lambda = 0$. This implies that the linearization in these coordinates takes a very suitable form with the linearized slow dynamics $\partial_t \delta x_1 = \epsilon \partial_x \Lambda \delta x_1$ exactly independent of the fast variables. \square

Note that

$$\|x_1 - x_0\|_{\chi, \nu} = \epsilon \|\phi_0 y\|_{\chi, \nu} \leq \epsilon \gamma_0 \sigma, \quad (3.3)$$

where $\sigma = \sup_{y \in \mathcal{V} + i\underline{\nu}} \|y\|$. From the linear equation (3.2) we immediately obtain

Lemma 3.1 *If $\epsilon \leq 1/(KC'_\Lambda)$ then the solution of (3.2) satisfies*

$$\|\phi_0\|_\chi \leq K\gamma_0. \quad \square$$

PROOF Take $\phi_0^0 = \mu A^{-1}$, let $r = \frac{K}{2}\gamma$ and introduce $\phi_0 = \phi_0^0 + z$ so that (3.2) becomes

$$z = F(z),$$

where $F(z) = \epsilon \partial_x \Lambda(\phi_0^0 + z)A^{-1}$. We have

$$\begin{aligned}\|F(z)\|_\chi &\leq \epsilon K C'_\Lambda r \leq r, \\ \|\partial_z F\|_\chi &\leq \frac{\epsilon K C'_\Lambda}{2} < 1.\end{aligned}$$

Here we have used the assumption $\epsilon \leq 1/(K C'_\Lambda)$. The function F is therefore a contraction on $B_r \subset \mathcal{V} + i\nu$ and there exists a unique solution of (3.2) with

$$\|\phi_0\|_\chi \leq 2r = K\gamma_0. \quad \blacksquare$$

Using this lemma we can then estimate the new error using a Cauchy estimate

$$\gamma_1 \equiv \|\mu_1\|_{\chi_1} \leq \epsilon \frac{K C_\Lambda}{\xi_0} \gamma_0,$$

where $\chi_1 = \chi - \xi_0$. We now use this result successively, introducing $x_n = x_{n+1} + \epsilon \phi_n(x_{n+1})y$ with ϕ_n solving

$$\epsilon \partial_x \Lambda \phi_n + \mu_n - \phi_n A = 0, \quad \mu_n = -\epsilon \partial_x \phi_{n-1} \Lambda, \quad (3.4)$$

on $x \in \mathcal{U} + i\chi_n$, $\chi_n = \chi - \sum_{i=0}^{n-1} \xi_i$, for each $n \geq 1$. We take $\xi_n = \xi = 2\epsilon K C_\Lambda$ at each step so that

$$\gamma_{n+1} \leq \epsilon \frac{K C_\Lambda}{\xi_n} \gamma_n \leq \frac{1}{2} \gamma_n \leq 2^{-(n+1)} \gamma_0,$$

with $\gamma_n = \|\mu_n\|_{\chi_n}$, $\chi_n = \chi - n\xi$. Note also that

$$\|x_n - x_0\|_{\chi_n, \nu} \leq \sum_{i=0}^{n-1} \|x_{i+1} - x_i\|_{\chi_n, \nu} \leq \epsilon \sigma \sum_{i=0}^{n-1} 2^{-i} \gamma_0 \leq 2\epsilon \sigma \gamma_0.$$

Setting $\chi_{N_\epsilon} = \underline{\chi}$ we realise that we can take $N_\epsilon = \frac{\chi - \underline{\chi}}{\xi} = \frac{\chi_0 - \underline{\chi}}{2\xi} = \mathcal{O}(\epsilon^{-1})$ steps so that

$$\gamma_{N_\epsilon} \leq 2^{-\left(\frac{\chi_0 - \underline{\chi}}{4\epsilon K C_\Lambda}\right)} \gamma_0.$$

Including $\rho = \mathcal{O}(e^{-C_1/\epsilon})$ does not change the conclusion. The result therefore follows.

Remark 3.2 Here we consider a fixed number applications of the SOF method, and show that the extension should only be iterated as many times as the first part has been iterated for the approximation of the slow manifold. To show this, we fix $k \in \mathbb{N}_0$, and apply the SO method k times to (1.2) so that the equations for $(x_0, y_k) = (x_0, y_0 - \eta^k(x_0))$ are

$$\begin{aligned}\partial_t x_0 &= \epsilon X_0(x_0, y_k + \eta^k), \\ \partial_t y_k &= \rho_k(x_0) + A_k(x_0)y_k + R_k(x_0, y_k),\end{aligned}$$

with $\rho_k = \mathcal{O}(\epsilon^{k+1})$. The SO method has then in fact been applied $k+1$ times to the original equations (1.1). Next, we apply the SOF method to these equations by introducing the transformation $x_0 = x_{n+1} + \epsilon\phi^n(x_{n+1})y_k$ where $\phi^n = \mathcal{O}(1)$ solves (2.4) with η replaced by η^k :

$$\begin{aligned}\partial_t x_{n+1} &= \epsilon X_{n+1}(x_{n+1}, y_k) \equiv \epsilon \left(X_0 - \phi^n \rho_n \right. \\ &\quad + \left\{ \epsilon(\partial_x X_0 + \partial_y X_0 \partial_x \eta^k) \phi^n - \epsilon \partial_x \phi^{n-1} X_0 + \partial_y X_0 - \phi^n (-\epsilon \partial_x \eta^k \partial_y X_0 + \partial_y Y_0) \right\} y_k \\ &\quad \left. - \epsilon \left(\partial_x (\phi^n - \phi^{n-1}) X_0 + \phi^n \partial_x \rho_k \phi^n \right) y_k + \mathcal{O}(y_k^2) \right) \\ &= \epsilon \left(X_0 - \phi^n \rho_n + \left(\epsilon \partial_x \phi_n X_0 + \epsilon \phi^n \partial_x \rho_k \phi^n \right) y_k + \mathcal{O}(y_k^2) \right).\end{aligned}$$

Here $\phi_n = \phi^n - \phi^{n-1} = \mathcal{O}(\epsilon^n)$ and X_0, Y_0 and their derivatives are all evaluated at $(x_0, \eta^k(x_0))$. Therefore the error, that is the term in X_{n+1} linear in y_k is formally of order

$$\epsilon \partial_x \phi_n X_0 + \epsilon \phi^n \partial_x \rho_k \phi^n = \mathcal{O}(\epsilon^{n+1}) + \mathcal{O}(\epsilon^{k+1}) = \mathcal{O}(\epsilon^{\min(n,k)+1}),$$

and, as expected, there is no improvement for n beyond k . A similar result holds true when considering the transformations in section 5 that seek to remove the terms in the slow vector field that are quadratic in the fast variables. \square

4 Michaelis-Menten-Henri model

In this section we demonstrate our method on the Michaelis-Menten-Henri model

$$\begin{aligned}\partial_t x_0 &= \epsilon X_0(x_0, y) = \epsilon(-x_0 + (x_0 + \kappa - \lambda)y), \\ \partial_t y &= Y(x_0, y) = x_0 - (x_0 + \kappa)y,\end{aligned}$$

for enzyme kinetics [31]. Here x_0 and y are non-negative concentrations and the parameters satisfy $\kappa > \lambda > 0$ and $0 < \epsilon \ll 1$. Setting $Y(x_0, y) = 0$ gives $y = \eta_0(x_0) = \frac{x_0}{x_0 + \kappa}$ and so $y = y_0 + \eta_0(x_0)$ transforms the system into

$$\begin{aligned}\partial_t x_0 &= \epsilon X_0(x_0, y_0) = \epsilon \left(-\frac{\lambda x_0}{x_0 + \kappa} + (x_0 + \kappa - \lambda)y_0 \right), \\ \partial_t y_0 &= Y_0(x_0, y_0) = \frac{\kappa \lambda x_0}{(x_0 + \kappa)^3} \epsilon - \left(x_0 + \kappa + \frac{\kappa(x_0 + \kappa - \lambda)}{(x_0 + \kappa)^2} \epsilon \right) y_0,\end{aligned}\tag{4.1}$$

Therefore if $\kappa \gg \epsilon$, so that

$$A_0 = \partial_y Y_0(x_0, 0) \equiv x_0 + \kappa + \frac{\epsilon \kappa (x_0 + \kappa - \lambda)}{(x_0 + \kappa)^2} \gg \epsilon,$$

x_0 being non-negative, then the system is slow-fast with $n_s = 1$ and $n_f = 1$. The variable x_0 is slow with $\partial_t x_0 = \mathcal{O}(\epsilon)$ and y_0 is fast with $(\partial_y Y_0)^{-1} = \mathcal{O}(1)$.

Analytic expressions of η and ϕ to $\mathcal{O}(\epsilon^2)$

We now obtain analytic expressions for η and ϕ . Since the model is actually linear in the fast variable the SOF method only involves the solution of linear equations. First, we introduce η_1 satisfying $Y_0(x_0, \eta_1) = 0$:

$$\eta_1(x) = \frac{\kappa \lambda x}{(x + \kappa)((x + \kappa)^3 + \epsilon \kappa(x + \kappa - \lambda))} \epsilon.$$

Then we define $Y_1(x_0, y_1) = -\partial_x \eta_0 X_0(x_0, \eta_1 + y_1) + Y_0(x_0, \eta_1 + y_1)$ and determine η_2 from the condition $Y_1(x_0, \eta_2) = 0$. We obtain

$$\eta_2 = \frac{x_0 (\kappa - 3x_0) \lambda^2 \kappa}{(x_0 + \kappa)^7} \epsilon^2 + \mathcal{O}(\epsilon^3),$$

and therefore

$$y_0 = \eta^2 = \eta_1 + \eta_2 = \frac{\kappa \lambda x_0}{(x_0 + \kappa)^4} \epsilon - \frac{\kappa \lambda x_0 (\kappa (\kappa - 2\lambda) + (\kappa + 3\lambda) x_0)}{(x_0 + \kappa)^7} \epsilon^2 + \mathcal{O}(\epsilon^3),$$

as a $\mathcal{O}(\epsilon^2)$ -approximation of the slow manifold.- The error-field is

$$\rho(x_0) = Y_2(x_0, 0) = \frac{\lambda^3 \kappa x_0 (\kappa^2 - 12\kappa x_0 + 15x_0^2)}{(x_0 + \kappa)^9} \epsilon^3 + \mathcal{O}(\epsilon^4). \quad (4.2)$$

To approximate the fiber directions we introduce y through $y_0 = \eta^2 + y$ and compute

$$\begin{aligned} \Lambda = X_0(x_0, \eta^2(x_0)) &= -\frac{\lambda x_0}{\kappa + x_0} + \frac{(\kappa - \lambda + x_0) \kappa \lambda x_0}{(\kappa + x_0)^4} \epsilon \\ &\quad - \frac{(\kappa - \lambda + x_0) \kappa \lambda x_0 (\kappa^2 - 2\kappa \lambda + (\kappa + 3\lambda) x_0)}{(\kappa + x_0)^7} \epsilon^2 + \mathcal{O}(\epsilon^3) \end{aligned} \quad (4.3)$$

$$\begin{aligned} A = \partial_y Y_0(x_0, \eta^2(x_0)) &= -\kappa - x_0 - \frac{\kappa (\kappa - \lambda + x_0)}{(\kappa + x_0)^2} \epsilon - \frac{(\kappa - 3x_0) (\kappa - \lambda + x_0) \kappa \lambda}{(\kappa + x_0)^5} \epsilon^2 \\ &\quad + \mathcal{O}(\epsilon^3), \end{aligned} \quad (4.4)$$

$$\mu_0 = x_0 + \kappa - \lambda.$$

Inserting this into (3.4) with $n = 0$ we obtain

$$\phi_0 = \frac{\mu_0}{A - \epsilon \partial_x \Lambda} = -\frac{x_0 + \kappa - \lambda}{x_0 + \kappa} + \frac{(x_0 + \kappa - \lambda) \kappa (x_0 - 2\lambda + \kappa)}{(x_0 + \kappa)^4} \epsilon + \mathcal{O}(\epsilon^2).$$

At the next step we first compute the new error

$$\mu_1 = -\epsilon \partial_x \phi_0 \Lambda = -\frac{\lambda^2 x_0}{(\kappa + x_0)^3} \epsilon + \mathcal{O}(\epsilon^2),$$

and via (3.4) with $n = 1$ we solve for ϕ_1

$$\phi_1 = \frac{\mu_1}{A - \epsilon \partial_x \Lambda} = \frac{\lambda^2 x_0}{(\kappa + x_0)^4} \epsilon + \mathcal{O}(\epsilon^2).$$

Then

$$\mu_2 = \frac{x_0 (\kappa - 3x_0) \lambda^3}{(\kappa + x_0)^6} \epsilon^2 + \mathcal{O}(\epsilon^3),$$

so that ϕ_2 via (3.4) with $n = 1$ becomes:

$$\phi_2 = -\frac{x_0 (\kappa - 3x_0) \lambda^3}{(x_0 + \kappa)^7} \epsilon^2 + \mathcal{O}(\epsilon^3).$$

Let $\phi^2 = \phi_0 + \phi_1 + \phi_2$:

$$\begin{aligned} \phi^2 = & -\frac{x_0 + \kappa - \lambda}{x_0 + \kappa} + \frac{(\kappa^3 - 3\kappa^2\lambda + 2x_0\kappa^2 - 3\kappa\lambda x_0 + x_0^2\kappa + 2\kappa\lambda^2 + \lambda^2x_0)}{(x_0 + \kappa)^4} \epsilon - (x_0 + \kappa)^{-7} \\ & \times \left(\kappa^2(-\lambda + \kappa)(6\lambda^2 - 6\kappa\lambda + \kappa^2) + \kappa(-\lambda + \kappa)(-2\lambda + \kappa)(-2\lambda + 3\kappa)x_0 \right. \\ & \left. + (-3\lambda^3 - \kappa^2\lambda + 3\kappa^3)x_0^2 + \kappa(\kappa + 3\lambda)x_0^3 \right) \epsilon^2 + \mathcal{O}(\epsilon^3). \end{aligned}$$

Then the span of the vector

$$\begin{aligned} v = & \begin{pmatrix} \epsilon\phi^2 \\ 1 + \epsilon\partial_x\eta^2\phi^2 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} + \begin{pmatrix} -\frac{(x_0 + \kappa - \lambda)}{x_0 + \kappa} \\ -\frac{(x_0 + \kappa - \lambda)\kappa}{(x_0 + \kappa)^3} \end{pmatrix} \epsilon \\ & + \begin{pmatrix} \frac{(\kappa(-\lambda + \kappa)(-2\lambda + \kappa) + (2\kappa - \lambda)(-\lambda + \kappa)x_0 + \kappa x_0^2)}{(x_0 + \kappa)^4} \\ \frac{(\kappa(-\lambda + \kappa)(\kappa - 3\lambda) + (2\kappa^2 - \kappa\lambda - 2\lambda^2)x_0 + (\kappa + 3\lambda)x_0^2)\kappa}{(x_0 + \kappa)^6} \end{pmatrix} \epsilon^2 + \mathcal{O}(\epsilon^3) \end{aligned}$$

gives a $\mathcal{O}(\epsilon^3)$ -approximation of the tangent space. We have left out the complicated $\mathcal{O}(\epsilon^3)$ -terms. The transformation $(x, y) \mapsto (x_0, y_0) = (x + \epsilon\phi^2y, y + \eta^2(x + \epsilon\phi^2y))$ transforms the system into:

$$\begin{aligned} \partial_t x &= \epsilon \left(\Lambda + \mu_3 y + \left(-\frac{(x + \kappa - \lambda)\lambda}{(x + \kappa)^2} \epsilon + \mathcal{O}(\epsilon^2) \right) y^2 + \mathcal{O}(\epsilon^2 y^3) \right), \\ \partial_t y &= \rho(x) + (A(x) + \mathcal{O}(\epsilon^4)) y + \mathcal{O}(\epsilon y^2), \end{aligned} \quad (4.5)$$

with

$$\mu_3 = -\frac{x\lambda^4(\kappa^2 - 12\kappa x + 15x^2)}{(x + \kappa)^9} \epsilon^3 + \mathcal{O}(\epsilon^4),$$

and where ρ , Λ and A are given in (4.2), (4.3) respectively (4.4).

Numerical computations of η and ϕ

In Fig. 2 (a) and (b) we have compared the solution (x_{0b}, y_{0b}) of (4.1) initiated at the base point $(x_{0b}^0, \eta(x_{0b}^0))$ with (i) the solution (x_0^i, y_0^i) initiated at $(x_{0b}^0, \eta(x_{0b}^0)) + v|v|^{-1}s$ (dashed)

and with (ii) (by the naive projection) the solution (x_0^{ii}, y_0^{ii}) initiated at $(x_{0b}^0, \eta(x_{0b}^0) + s)$ (full line) for different values of s and for a time integration of length $t = \epsilon^{-1}$. The parameter s measures the distance from the slow manifold and v is the tangent vector to the fiber at the base point $(x_{0b}^0, \eta(x_{0b}^0))$ determined through ϕ and the equation (2.3). We have set $\kappa = 2$, $\lambda = 1$ and $x_b^0 = 1.5$, and have computed η and ϕ numerically using the procedure described in Corollary 2.1. We have used 4 iterations on both η and ϕ resulting in error-fields of $\sim 10^{-7}$ respectively $\sim 10^{-10}$ for $\epsilon = 0.1$. The comparison is made through

$$\begin{aligned} v_i &= \|(x_{0b}, y_{0b})(\epsilon^{-1}) - (x_0^i, y_0^i)(\epsilon^{-1})\|, \\ \text{and} \\ v_{ii} &= \|(x_{0b}, y_{0b})(\epsilon^{-1}) - (x_0^{ii}, y_0^{ii})(\epsilon^{-1})\|. \end{aligned}$$

In (a) $\epsilon = 0.1$ while $\epsilon = 0.01$ in (b). We see that $v_i \ll v_{ii}$ and compute $v_i \approx \mathcal{O}(s^{2.009})$, whereas $v_{ii} \approx \mathcal{O}(s^{1.000})$.

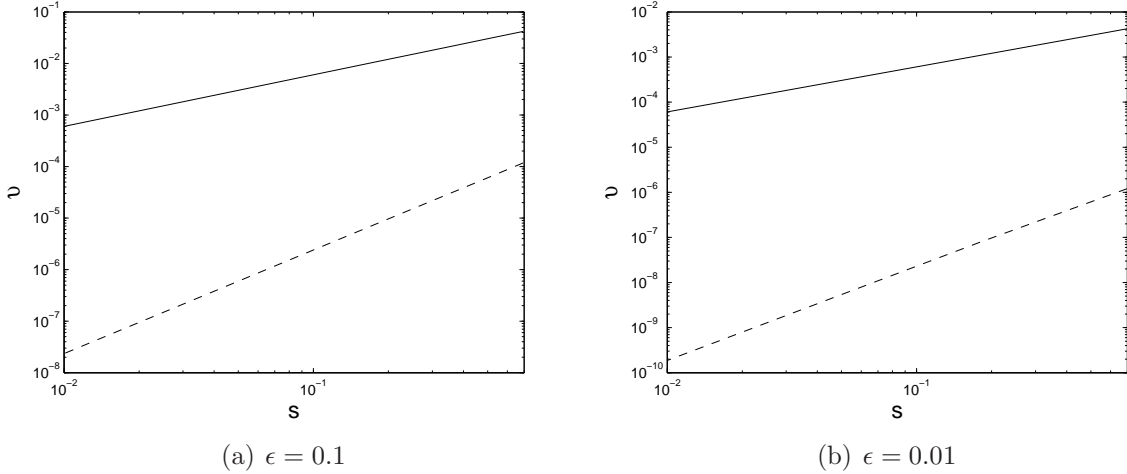


Figure 2: The errors from approximating fibers using the tangent spaces (v_i : dashed lines) and naive projections (v_{ii} : full lines) as functions of the distance from the slow manifold. Here $\kappa = 2$, $\lambda = 1$ and the initial condition on x_0 is $x_{0b}^0 = 1.5$.

The errors in η^n and ϕ^n :

$$\mathcal{E}_\eta = \sup_x |-\partial_x \eta X_0 + Y_0|,$$

respectively

$$\mathcal{E}_\phi = \sup_x |\epsilon(\partial_x X_0 + \partial_y X_0 \partial_x \eta) \phi - \epsilon \partial_x \phi X_0 + \partial_y X_0 - \phi(-\epsilon \partial_x \eta \partial_y X_0 + \partial_y Y_0)|,$$

for $\epsilon = 0.1$ are shown in Fig. 3 as a function of the iteration number. These are relevant errors since if $\mathcal{E}_\eta = 0$ then $y_0 = \eta$ is an exact slow manifold and if $\mathcal{E}_\phi = 0$ then the transformation $x_0 = x_1 + \epsilon \phi(x_1)y$ removes the term in $\partial_t x_1$ that is linear in y exactly. The error in ϕ and η are observed to be the order of machine precision $\sim 10^{-14}$ after 8 respectively 10 iterations. There is no or little improvement beyond this number. Note that this is in agreement with the

estimate of $N_\epsilon = \mathcal{O}(\epsilon^{-1}) \approx 10$ for $\epsilon = 0.1$. It should also be mentioned that to approximate derivatives we use the five-point stencil:

$$f'(x) \approx \frac{1}{2h}(-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)),$$

the error being $\frac{h^4}{30}f^{(5)}(x_0) = \mathcal{O}(h^4)$, $x_0 \in [x-2h, x+2h]$. We have used $h \approx 10^{-2}$ which gives an error of $\sim 10^{-8}$.

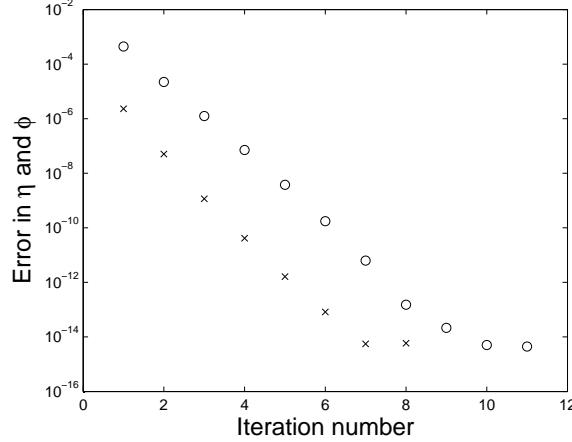


Figure 3: The errors \mathcal{E}_η (\circ) and \mathcal{E}_ϕ (\times) for $\epsilon = 0.1$ as a function of the iteration number. The functions η and ϕ are computed numerically using the recipe in Corollary 2.1. Here $\kappa = 2$, $\lambda = 1$ and the initial condition on x_0 is $x_{0b}^0 = 1.5$. In the computations leading to Fig. 2 we have used 4 iterations on both η and ϕ .

In Fig. 4 we have taken $s = 0.5$ and consider v_i and v_{ii} as functions of ϵ . Again, we see that $v_i \ll v_{ii}$ and compute $v_i \approx \mathcal{O}(\epsilon^2)$ whereas $v_{ii} \approx \mathcal{O}(\epsilon)$. This discrepancy is, however, exceptional as it is due to the fact that the Michaelis-Menten-Henri system is linear in the fast variable y_0 .

Finally, solutions (x_{0b}, y_{0b}) and (x_0^i, y_0^i) of (4.1) are shown in Fig. 5. The solution (x_0^i, y_0^i) is initiated on the fiber of the base point with $x_{0b}^0 = 1.5$, at a distance $s \approx 0.52$ from the base point. The full line near $y_0 = 0$ is the slow manifold. (x_{0b}, y_{0b}) and (x_0^i, y_0^i) at 9 different times are indicated by \times respectively \circ 's. For illustrative purposes we have chosen the relatively large value of $\epsilon = 0.4$. It is observed that, at least approximately, the solution (x_0^i, y_0^i) contracts along the fiber directions indicated by the dashed lines moving from upper left to lower right. The fiber directions are approximated as hyperplanes through ϕ .

5 Approximating the curvature of the fibers

In this section we show how the SOF method may be further extended to also approximate the curvature of the fibers. According to Theorem 2.1 and Corollary 1 the transformation

$$y \mapsto y_0 = y + \eta(x_0), \quad \tilde{x}_0 \mapsto x_0 = \tilde{x}_0 + \epsilon \phi(\tilde{x}_0)y,$$

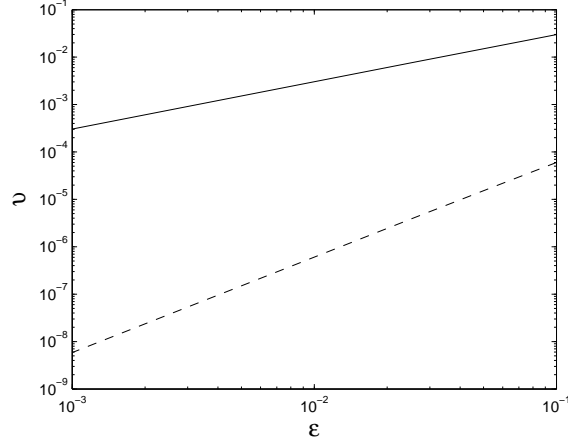


Figure 4: The errors from approximating fiber directions using the tangent spaces (dashed lines) and naive projections (full lines) as functions ϵ . Here $s = 0.5$, $\kappa = 2$, $\lambda = 1$ and the initial condition on x_0 is $x_{0b}^0 = 1.5$. We have used 4 iterations in the computations of η and ϕ .

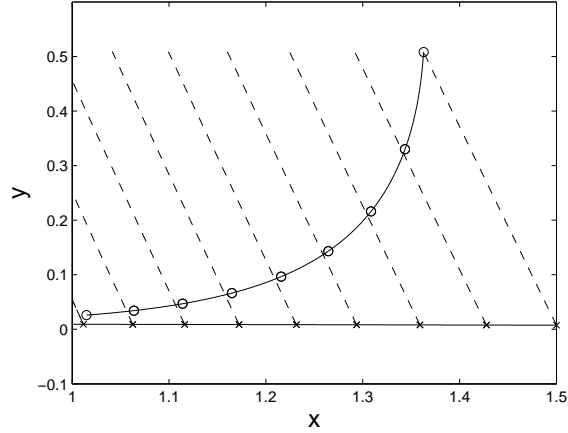


Figure 5: Solutions (x_{0b}, y_{0b}) and (x_0^i, y_0^i) of (4.1) for $\epsilon = 0.4$. The solution (x_0^i, y_0^i) is initiated on the fiber corresponding to the base point with $x_{0b}^0 = 1.5$, at a distance $s \approx 0.52$ from the base, and is observed to contract to the solution (x_{0b}, y_{0b}) along the fiber directions. The fiber directions are indicated by the dashed lines running from upper left to lower right.

transforms (2.1) into (2.2):

$$\begin{aligned}\partial_t \tilde{x}_0 &= \epsilon(\Lambda(\tilde{x}_0) + Q_0(\tilde{x}_0)y^2 + C(\tilde{x}_0, y)), \\ \partial_t y &= A(\tilde{x}_0)y + R(\tilde{x}_0, y),\end{aligned}\tag{5.1}$$

with $C = \mathcal{O}(y^3)$ and $R = \mathcal{O}(y^2)$ up to exponentially small error. We can easily obtain an explicit expression for the quadratic term $Q_0 y^2$, a vector of symmetric bilinear forms, in

terms of the known functions: X_0, Y_0, η and ϕ , through the equation $x_0 = \tilde{x}_0 + \epsilon\phi(\tilde{x}_0)y$. We will write the i th component of Q_0y^2 as

$$(Q_0y^2)_i = \langle y, Q_0^i y \rangle, \quad 1 \leq i \leq n_s,$$

where $Q_0^i = Q_0^i(x)$ is a symmetric $n_f \times n_f$ -matrix. Recall that we use the notation $(z)_i$ to denote the i th component of a vector z . Here we have also introduced the real inner product $\langle a, b \rangle = \sum_{i=1}^{n_f} (a)_i (b)_i$. By introducing

$$\tilde{x}_0 = \tilde{x}_1 + \epsilon\psi_0(\tilde{x}_1)y^2,$$

with ψ_0 a vector of symmetric bilinear forms, we therefore obtain

$$\partial_t \tilde{x}_1 = (I_s - \epsilon \partial_x \psi_0 y^2 + J^{-1}(\epsilon \partial_x \psi_0 y^2)^2) \epsilon (\Lambda + \{ \epsilon \partial_x \Lambda \psi_0 y^2 + Q_0 y^2 - 2\psi_0(y)(Ay) \} + \mathcal{O}(y^3)), \quad (5.2)$$

where $J = I_s + \epsilon \partial_x \psi_0 y^2$ is the Jacobian of the transformation $\tilde{x}_1 \mapsto \tilde{x}_0$. Here $\psi_0(y)(Ay)$ is understood as

$$(\psi_0(y)(Ay))_i = \frac{1}{2} \langle y, A^T \psi_0^i y \rangle + \frac{1}{2} \langle y, \psi_0^i A y \rangle.$$

The new error, that is the term in $\epsilon^{-1} \partial_t \tilde{x}_1$ which is quadratic in y , can again be decomposed into two separate contributions. One term comes from the expansion of $\partial_t \tilde{x}_0 - (\partial_y(\psi_0 y^2)) \partial_t y$, the curly bracket in (5.2), while the other one is due to the inverse of the Jacobian. As for the linear case, we choose the unknown function ψ_0 so that the curly bracket in (5.2) vanishes for all y . This gives

$$\epsilon \sum_{j=1}^{n_s} \partial_{(x)_j} (\Lambda)_i \psi_0^j + Q_0^i - A^T \psi_0^i - \psi_0^i A = 0. \quad (5.3)$$

By Theorem 4.4.6 in [10] this system has a unique solution ψ_0^i for $\epsilon = 0$ iff $\sigma(A) \cap \sigma(-A) = \emptyset$. Therefore we must exclude the elliptic case and the neutral saddle scenario where both λ and $-\lambda$, $\text{Re } \lambda \neq 0$, are eigenvalues of A . We consider this separately in section 6 below. Note moreover that by taking transposes:

$$Q_0^i - A^T (\psi_0^i)^T - (\psi_0^i)^T A = 0,$$

and so this solution is symmetric. The solution perturbs to a symmetric solution for $\epsilon \neq 0$ but small; $\epsilon \sum_{j=1}^{n_s} \partial_{(x)_j} (\Lambda)_i \psi_0^j$ is also symmetric. The solution satisfies

$$\|\psi_0\|_X \equiv \max_i \|\psi_0^i\|_X \leq \tilde{K} \|Q_0\|_X,$$

for some constant \tilde{K} depending on A^{-1} . Then the new error becomes

$$Q_1 = -\epsilon \partial_x \psi_0 \Lambda, \quad \|Q_1\|_{X-\xi} \leq \frac{\epsilon \tilde{K} C_\Lambda}{\xi} \|Q_0\|_X,$$

which also vanishes at exact equilibria where $\Lambda \equiv 0$. As for the linear case we have that $\Lambda_1 = \Lambda$ and $A_1 = A$. Using such transformations successively it is therefore possible to approximate the curvature of the fibers up to exponentially small error. Formally we proceed as in the proof of Theorem 2.1; the most important ingredient in the proof being the continued reduction of the domain together with the applications of Cauchy estimates to control the derivatives.

Theorem 5.1 *Assume that the assumptions of Theorem 2.1 hold true and that we have used the SOF method to transform (2.1) into (2.2). Assume furthermore that $\sigma(A) \cap \sigma(-A) = \emptyset$. Fix $0 \leq \underline{\underline{\chi}} < \underline{\chi}$. Then there exists an $\tilde{\epsilon}_0 \leq \epsilon_0$, where ϵ_0 is from Theorem 2.1, and an $\tilde{N}_\epsilon = \mathcal{O}(\epsilon^{-1}) \in \mathbb{N}$ so that for all $\epsilon \leq \tilde{\epsilon}_0$ the sequence of transformations $\tilde{x}_n = \tilde{x}_{n+1} + \epsilon \psi_n(\tilde{x}_{n+1})y^2$, $0 \leq n \leq \tilde{N}_\epsilon - 1$, where $\psi_n^i \in \mathbb{R}^{n_f \times n_f}$ solves*

$$\epsilon \sum_{j=1}^{n_s} \partial_{(x)_j}(\Lambda)_i \psi_n^j + Q_n^i - A^T \psi_n^i - \psi_n^i A = 0, \quad 1 \leq i \leq n_s, \quad (5.4)$$

the quantity

$$\epsilon Q_n y^2 = \begin{cases} \text{given by Eq. (5.1)} & \text{for } n = 0, \\ -\epsilon^2 \partial_x \psi_{n-1} \Lambda y^2 & \text{for } n \geq 1, \end{cases}$$

being the term in the expression for $\partial_t \tilde{x}_n$ which is quadratic in y , eventually transforms (2.2) into

$$\begin{aligned} \partial_t \tilde{x}_{\tilde{N}_\epsilon} &= \epsilon(\Lambda(\tilde{x}_{\tilde{N}_\epsilon}) + \tilde{C}(\tilde{x}_{\tilde{N}_\epsilon}, y)) + \mathcal{O}(e^{-\tilde{c}_1/\epsilon}), \\ \partial_t y &= A(\tilde{x}_{\tilde{N}_\epsilon})y + \tilde{R}(\tilde{x}_{\tilde{N}_\epsilon}, y) + \mathcal{O}(e^{-\tilde{c}_1/\epsilon}). \end{aligned} \quad (5.5)$$

Here $(\tilde{x}_{\tilde{N}_\epsilon}, y) \in (\mathcal{U} + i\underline{\underline{\chi}}) \times (\mathcal{V} + i\underline{\underline{\nu}})$, $\tilde{C} = \mathcal{O}(y^3)$ and

$$\|\tilde{C} - C\|_{\underline{\underline{\chi}}, \underline{\underline{\nu}}}, \|\tilde{R} - R\|_{\underline{\underline{\chi}}, \underline{\underline{\nu}}} \leq \tilde{c}_2 \epsilon,$$

for some constants \tilde{c}_1 and \tilde{c}_2 . Also the $\mathcal{O}(e^{-\tilde{c}_1/\epsilon})$ error terms in (5.5) vanish at true equilibria.

The transformation $(\tilde{x}, \tilde{y}) \mapsto (x, y) = (\tilde{x} + \epsilon \psi \tilde{y}^2, \tilde{y})$ with $\psi = \sum_{i=0}^{\tilde{N}_\epsilon-1} \psi_i$ differs from the product $(\tilde{x}_{\tilde{N}_\epsilon}, \tilde{y}) \mapsto \dots (\tilde{x}_1, y = \tilde{y}) \mapsto (\tilde{x}_0, y)$ by $\mathcal{O}(\tilde{y}^3)$ -terms and the equations for (\tilde{x}, \tilde{y}) therefore takes a similar form to (5.5): The set $\{\tilde{y} = 0\}$ is almost invariant and the \tilde{y} -space provides an almost $\mathcal{O}(\tilde{y}^2)$ -approximation to the fibers. In terms of the (x_0, y_0) -variables this quadratic approximation, parametrized by \tilde{y} , takes the following form:

$$\begin{aligned} x_0 &= \tilde{x} + \epsilon \phi \tilde{y} + \epsilon \psi \tilde{y}^2, \\ y_0 &= \tilde{y} + \eta + \partial_x \eta(\epsilon \phi \tilde{y} + \epsilon \psi \tilde{y}^2) + \frac{1}{2} \partial_x^2 \eta(\epsilon \phi \tilde{y})^2, \end{aligned}$$

for the base point $(\tilde{x}, \eta(\tilde{x}))$. □

Analytic expression of ψ to $\mathcal{O}(\epsilon^2)$ for the Michaelis-Menten-Henri model

We now apply this principle to the Michaelis-Menten-Henri model. We start from (4.5) where the quadratic term in $\epsilon^{-1} \partial_t x$ is of order $\mathcal{O}(\epsilon)$:

$$Q_1 = -\frac{(x + \kappa - \lambda) \lambda}{(x + \kappa)^2} \epsilon + \mathcal{O}(\epsilon^2).$$

We have therefore denoted this term by Q_1 rather than Q_0 . Then ψ_1 solves (5.4) with $n = 1$ and $\psi_0 = 0$:

$$\psi_1 = \frac{Q_1}{2A - \epsilon \partial_x \Lambda} = \frac{(x + \kappa - \lambda) \lambda}{2(x + \kappa)^3} \epsilon + \mathcal{O}(\epsilon^2),$$

so that

$$Q_2 = -\frac{\lambda^2 (2(x + \kappa) - 3\lambda) x}{2(x + \kappa)^5} \epsilon^2 + \mathcal{O}(\epsilon^3).$$

Finally

$$\psi_2 = \frac{\lambda^2 (2(x + \kappa) - 3\lambda) x}{4(x + \kappa)^6} \epsilon^2 + \mathcal{O}(\epsilon^3).$$

Let $\psi^2 = \psi_1 + \psi_2$:

$$\begin{aligned} \psi^2 &= \frac{(x + \kappa - \lambda) \lambda}{2(x + \kappa)^3} \epsilon + \frac{1}{4} (x + \kappa)^{-6} \left(2\kappa(-\lambda + \kappa)(8\lambda^2 - 9\kappa\lambda + 2\kappa^2) \right. \\ &\quad \left. + (38\kappa\lambda^2 - 44\kappa^2\lambda + 12\kappa^3 - 7\lambda^3)x + (4\lambda^2 + 12\kappa^2 - 22\kappa\lambda)\tilde{x}^2 + 4\kappa\tilde{x}^3 \right) + \mathcal{O}(\epsilon^3), \end{aligned}$$

then, in terms of the original (x_0, y) -variables, we have obtained the following quadratic $\mathcal{O}(\epsilon^2)$ -approximation of the fiber with base point $(\tilde{x}, \eta(\tilde{x}))$:

$$\begin{aligned} x_0 &= \tilde{x} + \epsilon \phi^2(\tilde{x}) \tilde{y} + \epsilon \psi^2(\tilde{x}) \tilde{y}^2 \\ &= \tilde{x} + \left(-\frac{(\tilde{x} + \kappa - \lambda)}{\tilde{x} + \kappa} \epsilon + \frac{\kappa(-\lambda + \kappa)(\kappa - 2\lambda) + (2\kappa - \lambda)(-\lambda + \kappa)\tilde{x} + \kappa\tilde{x}^2}{(\tilde{x} + \kappa)^4} \epsilon^2 + \mathcal{O}(\epsilon^3) \right) \tilde{y} \\ &\quad + \left(\frac{(\tilde{x} + \kappa - \lambda) \lambda}{2(\tilde{x} + \kappa)^3} \epsilon^2 + \mathcal{O}(\epsilon^3) \right) \tilde{y}^2, \\ y_0 &= \tilde{y} + \eta^2 + \partial_x \eta^2 (\epsilon \phi^2 \tilde{y} + \epsilon \psi^2 \tilde{y}^2) + \frac{1}{2} \partial_x^2 \eta^2 (\epsilon \phi^2 \tilde{y})^2 \\ &= \frac{\kappa \tilde{x} \lambda}{(\tilde{x} + \kappa)^4} \epsilon - \frac{\kappa \lambda \tilde{x} (\kappa^2 + \tilde{x} \kappa - 2\kappa \lambda + 3\lambda \tilde{x})}{(\tilde{x} + \kappa)^7} \epsilon^2 + \mathcal{O}(\epsilon^3) + \left(1 - \frac{(\tilde{x} + \kappa - \lambda)(\kappa - 3\tilde{x}) \kappa \lambda}{(\tilde{x} + \kappa)^6} \epsilon^2 \right. \\ &\quad \left. + \mathcal{O}(\epsilon^3) \right) \tilde{y} + \left(2 \frac{(\tilde{x} + \kappa - \lambda)(2\kappa - 3\tilde{x}) \kappa \lambda}{(\tilde{x} + \kappa)^7} \epsilon^2 + \mathcal{O}(\epsilon^3) \right) \tilde{y}^2, \end{aligned}$$

parametrized by \tilde{y} . We have here chosen only to show the $\mathcal{O}(\epsilon^2)$ -terms. In particular, $(x, y) = (\tilde{x} + \epsilon \psi^2(\tilde{x}) \tilde{y}^2, \tilde{y})$ transforms (4.5) into:

$$\begin{aligned} \partial_t \tilde{x} &= \epsilon (\Lambda(\tilde{x}) + \mu_3(\tilde{x}) \tilde{y} + Q_3 y^2 + \mathcal{O}(\epsilon^2 y^3)), \\ \partial_t \tilde{y} &= \rho(\tilde{x}) + (A(\tilde{x}) + \mathcal{O}(\epsilon^4)) \tilde{y} + \mathcal{O}(\epsilon y^2), \end{aligned}$$

with

$$Q_3 = \frac{(\tilde{x} + \kappa - \lambda) \kappa \lambda^2}{2(\tilde{x} + \kappa)^5} \epsilon^3 + \mathcal{O}(\epsilon^4).$$

Numerical computation of ψ

Fig. 6 shows the error

$$v = \|(x_b, y_b)(\epsilon^{-1}) - (\tilde{x}, \tilde{y})(\epsilon^{-1})\|$$

with (\tilde{x}, \tilde{y}) being the solution initiated at points along the quadratic approximation of the fibers with base (x_b, y_b) obtained from numerically computing the ψ_i 's, as a function of the distance $s \in [0.5, 10]$ ($s \sim \tilde{y}$) from the slow manifold. We have used 4 iterations in computing ψ giving rise to an error of $\sim 10^{-8}$ for $\epsilon = 0.1$. The error decreases as $\approx \mathcal{O}(s^{3.033})$ in agreement with the analysis.

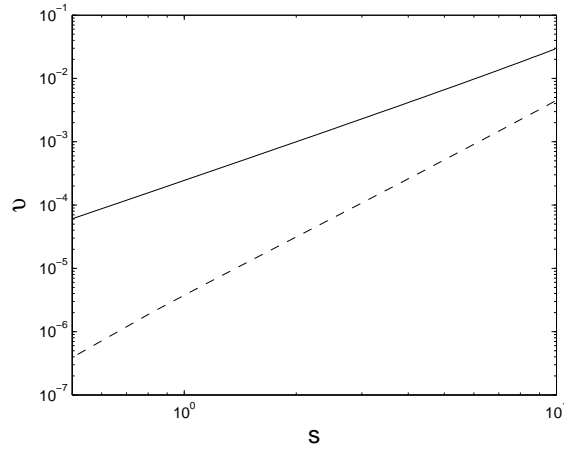


Figure 6: The error from approximating the fibers in the Michaelis-Menten-Henri model using a linear (full line) and quadratic (dashed line) approximation of the fiber as a function of the distance $s \in [0.5, 10]$ from the slow manifold. Here $\kappa = 2$, $\lambda = 1$, $\epsilon = 0.1$ and the initial condition on x is $x_b^0 = 1.5$. The error from the quadratic approximation decreases as $\approx \mathcal{O}(s^{3.033})$. We have used 4 iterations in the computations of η , ϕ and ψ .

6 Saddle type slow manifolds

Theorem 5.1 excludes the case of a neutral saddle type slow manifold. We proceed, as always in normal form calculations, by solving for what can be solved for, and therefore relax the requirements for the transformation. As before we are interested in a procedure described by simple equations and therefore choose not to use Fredholm's alternative to split the linear homological equations. We only aim to provide an outline for such a procedure here.

Assume that Theorem 2.1 has been applied and consider the equations

$$\begin{aligned}\partial_t \check{x}_0 &= \epsilon(\Lambda(\check{x}_0) + \mathcal{O}(\check{y}^2)), \\ \partial_t \check{y} &= A(\check{x}_0)\check{y} + \mathcal{O}(\check{y}^2),\end{aligned}$$

with $(\check{x}_0, \check{y}) \in (\mathcal{U} + i\underline{\chi}) \times (\mathcal{V} + i\underline{\nu})$ related to the old variables through the equations

$$\begin{aligned} x_0 &= \check{x}_0 + \epsilon \phi(\check{x}_0) \check{y}, \\ y_0 &= \eta(x_0) + \check{y}, \end{aligned}$$

and where exponentially small terms have been ignored. We assume that A has eigenvalues with positive and negative real parts. Before seeking to remove terms in the equation for \check{x}_0 that are quadratic in \check{y} , we first seek a splitting of \check{y} into “stable and unstable parts”. To do so we first perform a change of basis

$$\check{y} = V(\check{x}_0) \check{y}_0, \quad A_0 \equiv V^{-1} A V = \begin{pmatrix} A_{s0} & 0 \\ 0 & A_{u0} \end{pmatrix},$$

where $\sigma(A_{s0}) \subset (-\infty, -\underline{\lambda}]$, $\sigma(A_{u0}) \subset [\underline{\lambda}, \infty)$ for some $\underline{\lambda} > 0$, so that

$$\begin{aligned} \partial_t \check{x}_0 &= \epsilon(\Lambda + \mathcal{O}(y_0^2)), \\ \partial_t \check{y}_0 &= (A_0 + \epsilon B_0) \check{y}_0 + \mathcal{O}(\check{y}_0^2), \quad B_0 = -V^{-1} \partial_x V \Lambda. \end{aligned}$$

We then apply transformations of the form

$$\check{y}_i = (I_f + \epsilon \varphi_i) \check{y}_{i+1},$$

where $\varphi_i(\check{x}_0) \in \mathbb{R}^{n_f \times n_f}$ for $\check{x}_0 \in \mathcal{U}$, to remove the off block diagonal terms of the resulting B_i 's. Let us consider the first step. Introducing $\check{y}_0 = (I_f + \epsilon \varphi_0) \check{y}_1$ gives

$$\begin{aligned} \partial_t \check{y}_1 &= (I_f + \epsilon \varphi_0)^{-1} (\partial_t \check{y}_0 - \epsilon^2 \partial_x \varphi_0 \Lambda \check{y}_1 + \mathcal{O}(\check{y}_1^2)) \\ &= \left\{ (I_f + \epsilon \varphi_0)^{-1} (A_0 + \epsilon B_0) (I_f + \epsilon \varphi_0) \right\} \check{y}_1 \\ &\quad - \epsilon^2 (I_f + \epsilon \varphi_0)^{-1} \partial_x \varphi_0 \Lambda \check{y}_1 + \mathcal{O}(\check{y}_1^2). \end{aligned} \tag{6.1}$$

Set $J_f = I_f + \epsilon \varphi_0$ and introduce the following splitting of B_0

$$\begin{aligned} B_0 &= \begin{pmatrix} B_{s0} & B_{su0} \\ B_{us0} & B_{u0} \end{pmatrix} = B_{01} + B_{02}, \\ B_{01} &= \begin{pmatrix} B_{s0} & 0 \\ 0 & B_{u0} \end{pmatrix}, \quad B_{02} = \begin{pmatrix} 0 & B_{su0} \\ B_{us0} & 0 \end{pmatrix}. \end{aligned}$$

We will collect the block diagonal parts B_{01} and A_0 into $A_1 = \begin{pmatrix} A_{s1} & 0 \\ 0 & A_{u1} \end{pmatrix} = A_0 + \epsilon B_{01}$ with $A_{s1} = A_{s0} + \epsilon B_{s0}$, $A_{u1} = A_{u0} + \epsilon B_{u0}$, and seek to remove B_{02} . For this we expand the matrix shown with curly brackets in (6.1):

$$\begin{aligned} J_f^{-1} (A_0 + \epsilon B_0) J_f &= (I_f - \epsilon \varphi_0 + \epsilon^2 J_f^{-1} \varphi_0^2) (A_0 + \epsilon B_0) (I_f + \epsilon \varphi_0) \\ &= A_1 + \epsilon \{A_0 \varphi_0 - \varphi_0 A_0 + B_{02}\} \\ &\quad + \epsilon^2 (B_0 \varphi_0 - \varphi_0 B_0 - \varphi_0 (A_0 + \epsilon B_0) \varphi_0 + J_f^{-1} \varphi_0^2 (A_0 + \epsilon B_0) J_f). \end{aligned} \tag{6.2}$$

We then pick φ_0 of the form

$$\varphi_0 = \begin{pmatrix} 0 & \varphi_{su0} \\ \varphi_{us0} & 0 \end{pmatrix},$$

so that the curly bracket in (6.2) becomes

$$\begin{pmatrix} A_{s0} & 0 \\ 0 & A_{u0} \end{pmatrix} \varphi_0 - \varphi_0 \begin{pmatrix} A_{s0} & 0 \\ 0 & A_{u0} \end{pmatrix} + B_{02} = \begin{pmatrix} 0 & A_{s0}\varphi_{su0} - \varphi_{su0}A_{u0} + B_{su0} \\ A_{u0}\varphi_{us0} - \varphi_{us0}A_{s0} + B_{us0} & 0 \end{pmatrix},$$

which we set to zero:

$$A_{s0}\varphi_{su0} - \varphi_{su0}A_{u0} + B_{su0} = 0, \quad A_{u0}\varphi_{us0} - \varphi_{us0}A_{s0} + B_{us0} = 0.$$

These equations are solvable for φ_{su0} respectively φ_{us0} since by assumption we have $\sigma(A_{s0}) \cap \sigma(A_{u0}) = \emptyset$. Also the solutions satisfy

$$\|\varphi_{su0}\|_{\underline{\chi}}, \|\varphi_{us0}\|_{\underline{\chi}} \leq \check{K} \|B_{02}\|_{\underline{\chi}}, \quad (6.3)$$

for some constant \check{K} . The new error

$$B_1 = \epsilon (B_0\varphi_0 - \varphi_0 B_0 - \varphi_0(A_0 + \epsilon B_0)\varphi_0 + J^{-1}\varphi_0^2(A_0 + \epsilon B_0)J) - \epsilon J^{-1}\partial_x \varphi_0 \Lambda,$$

is $\mathcal{O}(\epsilon)$. Through (6.3) and a Cauchy estimate for the derivate $\partial_x \varphi_0$, this error can in fact directly be estimated by $\xi^{-1}\check{C}\|B_{02}\|_{\underline{\chi}}$ on the smaller domain $\mathcal{U} + i(\underline{\chi} - \xi)$ for some constant $\check{C} > 0$. We then again argue that for ϵ sufficiently small we will after $\check{N}_\epsilon = \mathcal{O}(\epsilon^{-1})$ steps of this procedure have that $B_{\check{N}_\epsilon} = \mathcal{O}(e^{-c/\epsilon})$.

We then continue by considering $\check{y}_{\check{N}_\epsilon} = (\check{y}_s, \check{y}_u)$ and the equations

$$\begin{aligned} \partial_t \check{x}_0 &= \epsilon(\Lambda(\check{x}_0) + Q_{s0}(\check{x}_0)\check{y}_s^2 + Q_{u0}(\check{x}_0)\check{y}_u^2 + Q_{us}(\check{x}_0)(\check{y}_s)(\check{y}_u) + \mathcal{O}(3)), \\ \partial_t \check{y}_s &= A_s(\check{x}_0)\check{y}_s + \mathcal{O}(2), \\ \partial_t \check{y}_u &= A_u(\check{x}_0)\check{y}_u + \mathcal{O}(2), \end{aligned} \quad (6.4)$$

where $\mathcal{O}(2)$ and $\mathcal{O}(3)$ denote terms that are quadratic respectively cubic in $\check{y}_{\check{N}_\epsilon}$ and where we have ignored the exponentially small terms. The eigenvalues of A_s all have negative real parts while the eigenvalues of A_u all have positive real parts. In accordance with (1.7), we will now aim to remove the terms in the equation for \check{x}_0 that are quadratic in y_s and y_u ; to avoid small divisors completely we will not seek to remove terms of the form $Q_{su}(y_s)(y_u)$. We therefore apply the following transformation to the slow variables:

$$\check{x}_0 = \check{x}_1 + \epsilon\psi_{s0}\check{y}_s^2 + \epsilon\psi_{u0}\check{y}_u^2, \quad (6.5)$$

to push the current errors Q_{s0} and Q_{u0} to higher order in ϵ . We obtain:

$$\begin{aligned} \partial_t \check{x}_1 &= J^{-1}\epsilon \left(\Lambda + \left\{ \epsilon \partial_x \Lambda(\psi_{s0}\check{y}_s^2 + \psi_{u0}\check{y}_u^2) + Q_{s0}\check{y}_s^2 + Q_{u0}\check{y}_u^2 \right. \right. \\ &\quad \left. \left. - 2\psi_{s0}(\check{y}_s)(A_s\check{y}_s) - 2\psi_{u0}(\check{y}_u)(A_u\check{y}_u) \right\} + Q_{us}(\check{y}_s)(\check{y}_u) + \mathcal{O}(3) \right). \end{aligned}$$

Here we have suppressed the dependency on \check{x}_1 and by $J = I_s + \epsilon \partial_x \psi_{s0} \check{y}_s^2 + \epsilon \partial_x \psi_{u0} \check{y}_u^2$ denoted the Jacobian of the transformation $\check{x}_1 \mapsto \check{x}_0$. Again we set the curly brackets to zero:

$$\epsilon \partial_x \Lambda (\epsilon \psi_{s0} \check{y}_s^2 + \epsilon \psi_{u0} \check{y}_u^2) + Q_{s0} \check{y}_s^2 + Q_{u0} \check{y}_u^2 - \psi_{s0}(\check{y}_s)(A_s \check{y}_s) - \psi_{u0}(\check{y}_u)(A_u \check{y}_u) = 0$$

for all $y = (\check{y}_s, \check{y}_u)$. As in (5.4), this gives

$$\begin{aligned} \epsilon \sum_{j=1}^{n_s} \partial_{(x)_j}(\Lambda)_i \psi_{s0}^j + Q_{s0}^i - A_s^T \psi_{s0}^i - \psi_{s0}^i A_s &= 0, \quad 1 \leq i \leq n_s, \\ \epsilon \sum_{j=1}^{n_s} \partial_{(x)_j}(\Lambda)_i \psi_{u0}^j + Q_{u0}^i - A_u^T \psi_{u0}^i - \psi_{u0}^i A_u &= 0, \quad 1 \leq i \leq n_s. \end{aligned}$$

These equations are solvable for ϵ sufficiently small as by assumption $\sigma(A_s) \cap \sigma(-A_s) = \emptyset = \sigma(A_u) \cap \sigma(-A_u)$. The new errors are therefore

$$Q_{s1} = -\epsilon \partial_x \psi_{s0} \Lambda, \quad Q_{u1} = -\epsilon \partial_x \psi_{u0} \Lambda,$$

which are due to the inverse of the Jacobian. They again vanish at true equilibria where $\Lambda \equiv 0$. We iterate the procedure and apply Cauchy estimates to conclude that the errors are eventually exponentially small. The stable fiber of the invariant slow manifold $\{\check{y}_s = 0, \check{y}_u = 0\}$ then coincides with $\{\check{y}_u = 0\}$ while the unstable fiber coincides with $\{\check{y}_s = 0\}$ up to terms cubic in \check{y}_s and \check{y}_u and exponentially small terms. These spaces can through the functions ϕ_i , φ_i , ψ_{si} and ψ_{ui} be described in terms of the original variables.

7 Conclusion

In this paper we developed a new method, the SOF method, as an extension of the method of straightening out (SO method) so that it can also be used to approximate fiber directions. The method is based on normal form computations. After having approximated the slow manifold using the SO method, the extended method constructs a transformation of the slow variables as a product of a finite sequence of transformations, each obtained as the solution of a linear equation, so that the slow dynamics becomes almost independent of the fast variable to linear order. See Theorem 2.1. This gives an approximation, with exponentially small error, of the tangent spaces of the fibers. The method is easily implemented numerically as it only involves evaluations of the initial vector-field and its Jacobian matrix. See Corollary 1. The method was also extended further in Theorem 5.1 so that it approximates, again exponentially well, the curvature of the fibers. This result holds true even when the slow manifold is of saddle type. In the saddle case, we only require that it is not neutral in the sense that there does not exist a contraction and an expansion rate of equal magnitude. For this scenario we followed the general philosophy of normal form theory and solved for what could be solved for. In agreement with Fenichel's normal form, we were able to construct a procedure, valid for any saddle type slow manifold not just the neutral ones, that removed terms in the slow vector field that were quadratic in the fast variables associated with the contraction respectively the fast variables associated with the expansion from the slow manifold up to exponential small error.

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